TMA4255 Applied Statistics
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*
Factorial Experiments at Two Levels

Bo Lindqvist

The note is adapted from the note
Tyssedal: “To-nivå faktorielle forsøk og blokkdeling”.

Example

The connection between yield of a chemical process and the two factors temperature and concentration is to be investigated. Four experiments are conducted, where two values of each factor are used. This gives 4 possible level combinations of the two factors to investigate the yield. The experiment is given in the table below, where the observed responses (yield) are also given:

Experiment no.	Temperature	Concentration	Yield
1	160	20	60
2	180	20	72
3	160	40	54
4	180	40	68
	x_1	x_2	y

The appropriate linear regression model is

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_{12} x_1 x_2 + \epsilon,$$

where the product term $x_1 x_2$ is included in order to model a possible interaction between the two factors temperature and concentration.

The design matrix X of this model is obviously:

$$X = \begin{bmatrix} 1 & 160 & 20 & 3200 \\ 1 & 180 & 20 & 3600 \\ 1 & 160 & 40 & 6400 \\ 1 & 180 & 40 & 7200 \end{bmatrix}$$

MINITAB fits the following model:

```
Regression Analysis: y versus x1; x2; x1x2

The regression equation is
y = - 14,0 + 0,500 x1 - 1,10 x2 + 0,00500 x1x2

Predictor        Coef
Constant     -14,0000
x1           0,500000
x2           -1,10000
x1x2       0,00500000
```

Let us now recode the factors by introducing new independent variables

$$\begin{aligned} z_1 &= \frac{x_1 - 170}{10} \\ z_2 &= \frac{x_2 - 30}{10} \\ z_{12} &= z_1 \cdot z_2 \end{aligned}$$

The regression model is now

$$y = \beta_0 + \beta_1 z_1 + \beta_2 z_2 + \beta_{12} z_{12} + \epsilon \tag{1}$$

with design matrix

$$X = \begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \tag{2}$$

and MINITAB finds the following model:

```
Regression Analysis: y versus z1; z2; z12

The regression equation is
y = 63,5 + 6,50 z1 - 2,50 z2 + 0,500 z12

Predictor        Coef
Constant      63,5000
z1            6,50000
z2           -2,50000
z12          0,500000
```

To see that we have the same fitted model, we can substitute the expressions for z_1, z_2, z_{12} in terms of the x_1, x_2, to get:

$$\begin{aligned} \hat{y} &= 63.5 + 6.5 \cdot \frac{x_1 - 170}{10} - 2.5 \cdot \frac{x_2 - 30}{10} + 0.5 \cdot \frac{x_1 - 170}{10} \cdot \frac{x_2 - 30}{10} \\ &= -14 + 0.5x_1 - 1.1x_2 + 0.005x_1x_2 \end{aligned}$$

Design of Experiments (DOE) terminology

In the example we consider two *factors*, A=temperature, B=concentration, and the response y=yield.

Each factor has two levels:

Factor	low	high
A	160^o (-1)	180^o (+1)
B	20^o (-1)	40^o (+1)

We have thus 2 factors which each can be on 2 levels, making $2^2 = 4$ possible combinations. The following is standard notation of such an experiment, a so called 2^2 experiment:

A	B	AB	Level code	Response
-1	-1	1	1	y_1
1	-1	-1	a	y_2
-1	1	-1	b	y_3
1	1	1	ab	y_4
z_1	z_2	z_{12}		

The level code shows the factor(s) at high level for the corresponding level combination.

Multivariate regression with orthogonal design matrix X (Chapter 12.7 in book)

Consider the vector/matrix setup $y = X\beta + \epsilon$, or written out,

$$\begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix} = \begin{bmatrix} 1 & x_{11} & x_{21} & \cdots & x_{k1} \\ 1 & x_{12} & x_{22} & \cdots & x_{k2} \\ \vdots & & & & \\ 1 & x_{1n} & x_{2n} & \cdots & x_{kn} \end{bmatrix} \begin{bmatrix} \beta_0 \\ \beta_1 \\ \vdots \\ \beta_k \end{bmatrix} + \begin{bmatrix} \epsilon_1 \\ \epsilon_2 \\ \vdots \\ \epsilon_n \end{bmatrix}$$

We say that X has orthogonal columns if the product-sum of any two columns is 0. This means here that:

$$\sum_{i=1}^{n} x_{ji}x_{\ell i} = 0 \text{ when } j \neq \ell \ (j, \ell = 1, \ldots, k)$$

$$\sum_{i=1}^{n} x_{\ell i} = 0 \text{ for } \ell = 1, \ldots, k$$

The last equality, which says that each of the column sums for $\ell = 1, \ldots, k$ are 0, follows since the left column has only 1s).

A remarkable fact about the estimated regression coefficients in the above model is that each b_j depends on X only via the corresponding column for x_j, and that the estimated coefficients hence do not change when we look at submodels (i.e. take out variables from the model). The formulas are:

$$\begin{aligned} b_0 &= \bar{y} \\ b_j &= \frac{\sum_{i=1}^{n} x_{ji}y_i}{\sum_{i=1}^{n} x_{ji}^2} \text{ for } j = 1, 2, \ldots, k \end{aligned} \tag{3}$$

from which we get in particular

$$Var(b_j) = \frac{\sigma^2}{\sum_{i=1}^{n} x_{ji}^2} \quad \text{(prove it!)}$$

We also have:

$$SSR = b_1^2 \sum_{i=1}^{n} x_{1i}^2 + b_2^2 \sum_{i=1}^{n} x_{2i}^2 + \cdots + b_k^2 \sum_{i=1}^{n} x_{ki}^2 \tag{4}$$

so that

$$SSE = SST - SSR = \sum_{i=1}^{n} (y_i - \bar{y})^2 - b_1^2 \sum_{i=1}^{n} x_{1i}^2 - \cdots - b_k^2 \sum_{i=1}^{n} x_{ki}^2$$

Back to the 2^2 experiment

We see that the columns of X in (2) are orthogonal (check!) This simplifies the estimation of the regression coefficients. Here we can use the formulas (3). Note that all the x_{ji} are now equal to ± 1, so $\sum_{i=1}^{n} x_{ji}^2 = n(=4)$, and the numerators are all of the form $\sum_{i=1}^{n} \pm y_i$ where $+$ or $-$ are determined from the corresponding colums. Such expressions are called *contrasts.*

We get, using the formula in (3):

$$\begin{aligned}
b_0 &= \frac{y_1+y_2+y_3+y_4}{4} = 63.5 \\
b_1 &= \frac{-y_1+y_2-y_3+y_4}{4} = \frac{y_2+y_4}{4} - \frac{y_1+y_3}{4} = 6.5 \\
b_2 &= \frac{-y_1-y_2+y_3+y_4}{4} = \frac{y_3+y_4}{4} - \frac{y_1+y_2}{4} = -2.5 \\
b_{12} &= \frac{y_1-y_2-y_3+y_4}{4} = \frac{y_4-y_3}{4} - \frac{y_2-y_1}{4} = 0.5
\end{aligned}$$

These estimators can be given an interpretation using Design of Experiments (DOE) terminology:

First, b_0 is named *mean response.*

Note that when factor A goes from low level (-1) to high level (+1), the mean response of y increases by $2\beta_1$ (see the regression model (1)). This is interpreted as the *main effect of A*. Therefore, the estimate $2b_1$ will be interpreted as the estimated main effect of A, denoted $\hat{A}$. The following gives a nice and intuitive interpretation of $\hat{A}$, where the last line is used as a general definition of the main effect of a factor in DOE.

$$\begin{aligned}
\hat{A} &= 2b_1 \\
&= \frac{y_2+y_4}{2} - \frac{y_1+y_3}{2} \\
&= \text{mean response when A is high} \;-\; \text{mean response when A is low}
\end{aligned}$$

Similarly, the estimated effect of B is:

$$\begin{aligned}
\hat{B} &= 2b_2 \\
&= \frac{y_3+y_4}{2} - \frac{y_1+y_2}{2} \\
&= \text{mean response when B is high} \;-\; \text{mean response when B is low}
\end{aligned}$$

Now what is the DOE interpretation corresponding to b_{12}? The answer is that $2b_{12}$ is denoted $\widehat{AB}$ and called the *estimated interaction effect between A and B.* We have the following motivation for this, where the last line is the general definition of a two-factor interaction:

$$\begin{aligned}
\widehat{AB} &= 2b_{12} \\
&= \frac{y_4-y_3}{2} - \frac{y_2-y_1}{2} \\
&= \frac{\text{estimated main effect of A when B is high}}{2} \\
&- \frac{\text{estimated main effect of A when B is low}}{2}
\end{aligned}$$

Note that we also have the symmetric interpretation:

$$\begin{aligned}
\widehat{AB} &= 2b_{12} \\
&= \frac{y_4 - y_2}{2} - \frac{y_3 - y_1}{2} \\
&= \frac{\text{estimated main effect of B when A is high}}{2} \\
&- \frac{\text{estimated main effect of B when A is low}}{2}
\end{aligned}$$

From this we compute:

$$\begin{aligned}
\hat{A} &= \frac{72 + 68}{2} - \frac{60 + 54}{2} = 13 \\
\hat{B} &= \frac{54 + 68}{2} - \frac{60 + 72}{2} = -5 \\
\widehat{AB} &= \frac{68 - 54}{2} - \frac{72 - 60}{2} = 1
\end{aligned}$$

Figure 1 illustrates the estimates.

Three factors

The standard setup is as follows, where + corresponds to high level and - corresponds to low level of the factors.

A	B	C	AB	AC	BC	ABC	Level code	Response
-	-	-	+	+	+	-	1	60
+	-	-	-	-	+	+	a	72
-	+	-	-	+	-	+	b	54
+	+	-	+	-	-	-	ab	68
-	-	+	+	-	-	+	c	52
+	-	+	-	+	-	-	ac	83
-	+	+	-	-	+	-	bc	45
+	+	+	+	+	+	+	abc	80
z_1	z_2	z_3	z_{12}	z_{13}	z_{23}	z_{123}		

The corresponding regression model is:

$$y = \beta_0 + \beta_1 z_1 + \beta_2 z_2 + \beta_3 z_3 + \beta_{12} z_{12} + \beta_{13} z_{13} + \beta_{23} z_{23} + \beta_{123} z_{123} + \epsilon$$

where $z_{12} = z_1 z_2$, $z_{13} = z_1 z_3$, $z_{23} = z_2 z_3$, $z_{123} = z_1 z_2 z_3$ and the design matrix is given by putting -1 instead of $-$, $+1$ instead of $+$ and adding a column of 1s to the left in the table above.

Estimated effects using the above data are given on slides from the lectures. While the main effects $\hat{A}$, $\hat{B}$ are straightforward to compute, we now have, for example,

$$\begin{aligned}
\widehat{AB} &= 2b_{12} \\
&= \frac{\text{estimated main effect of A when B is high}}{2}
\end{aligned}$$

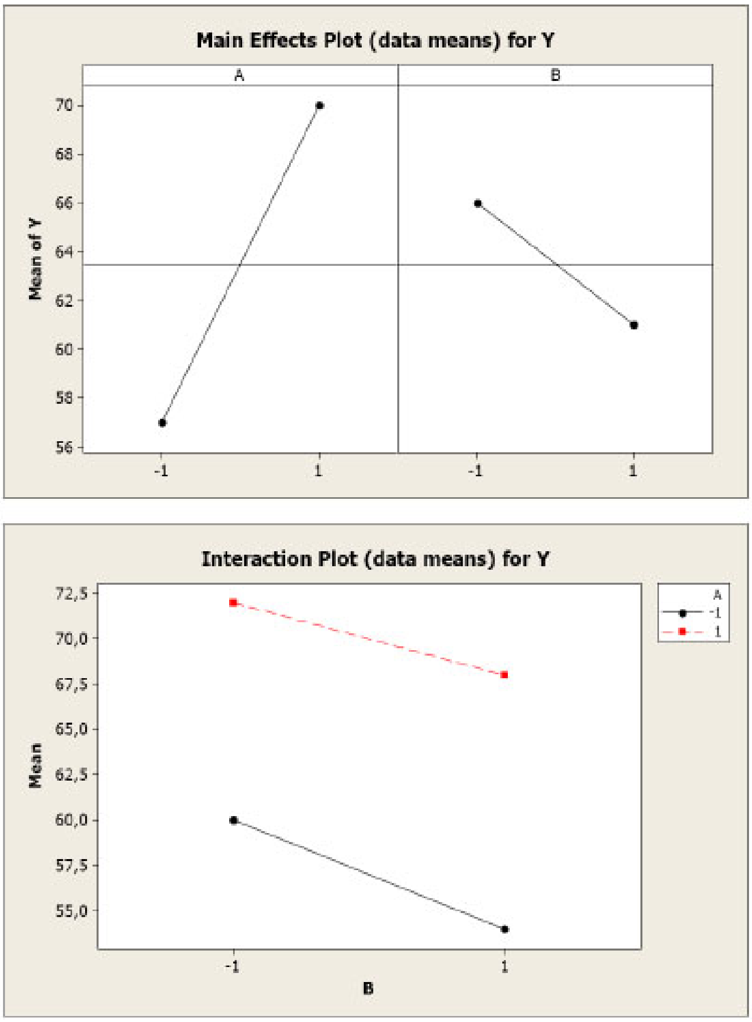


Figure 1: Graphical representation of estimated main effects and interaction in 2^2 experiment

$$
\begin{aligned}
&- \frac{\text{estimated main effect of A when B is low}}{2} \\
&= \frac{\frac{68+80}{2} - \frac{45+54}{2}}{2} - \frac{\frac{83+72}{2} - \frac{52+60}{2}}{2} \\
&= 1.5
\end{aligned}
$$

A brand new concept is the estimated third order interaction between A, B and C. This is defined and interpreted as follows:

$$
\begin{aligned}
\widehat{ABC} &= 2b_{123} \\
&= \frac{\text{estimated interaction between A and B when C is high}}{2} \\
&- \frac{\text{estimated interaction between A and B when C is low}}{2}
\end{aligned}
$$

You should check yourself that this is the same as computing $2b_{123}$ by using the + and - in the column of ABC in the given table. Also check that we may write "A and C when B is high/low" or "B and C when A is high/low" and get the same result for $\widehat{ABC}$.

General full factorial 2^k experiment

In general there are k factors, usually named A,B,C,D,E,... which each can be at two levels. The regression model can be written

$$
\begin{aligned}
y &= \beta_0 + \beta_1 z_1 + \beta_2 z_2 + \cdots + \beta_k z_k \\
&+ \beta_{12} z_{12} + \beta_{13} z_{13} + \cdots + \beta_{k-1,k} z_{k-1,k3} \\
&+ \beta_{123} z_{123} + \cdots + \beta_{k-2,k-1,k} z_{k-2,k-1,k} \\
&+ \cdots \\
&+ \beta_{123\cdots k} z_{123\cdots k} \\
&+ \epsilon
\end{aligned}
$$

Here 1 corresponds to A, 2 corresponds to B, 12 corresponds to AB, etc. There are k main effects (single indices), $\left(\begin{array}{c} k \\ 2 \end{array}\right)$ two-factor interactions, $\left(\begin{array}{c} k \\ 3 \end{array}\right)$ third order interactions, etc. Hence there are altogether (including β_0)

$$
1 + \left(\begin{array}{c} k \\ 2 \end{array}\right) + \left(\begin{array}{c} k \\ 2 \end{array}\right) + \cdots \left(\begin{array}{c} k \\ 2 \end{array}\right) = 2^k
$$

coefficients in the model. It can be shown that the design matrix is, for any k, orthogonal. Thus we have the simple estimates of the coefficients given by

$$
b_j = \frac{\sum_{i=1}^n x_{ji} y_i}{\sum_{i=1}^n x_{ji}^2} = \frac{\sum_{i=1}^n \pm y_i}{n}
$$

so that the corresponding effect is given by

$$
\widehat{Effect}_j = 2b_j = \frac{\sum_{i=1}^n \pm y_i}{\frac{n}{2}}
$$

where the $+$ and $-$ in front of the y_i are determined from the corresponding column in the factor table, and n is the number of observations. Here and later we will use $\widehat{Effect}_j$ to denote a generic estimated effect, which in practice can be any of $\hat{A}$, $\widehat{AB}$, $\widehat{ABC}$ etc. The index j may also correspond to interactions, for example $j = (123)$ for interaction between A,B and C. It will also sometimes be convenient to define $Effect_j$ without hat to mean simply $2\beta_j$ (for main effects or interactions).

It follows, since the y all have the same variance σ^2, that for any estimated effect:

$$Var(\widehat{Effect}_j) = Var(\frac{\sum_{i=1}^{n} \pm y_i}{\frac{n}{2}}) = \frac{n\sigma^2}{\frac{n^2}{4}} = \frac{4\sigma^2}{n} \equiv \sigma^2_{effect}$$

The quantity σ^2_{effect} has here been introduced for convenience. We will use it interchangeably with σ^2. The two should not be confused.

Estimation of σ^2

In multiple regression we used

$$s^2 = \frac{SSE}{n - r - 1}$$

where r is the number of independent variables. In a full factorial 2^k experiment we have $r = 2^k - 1$ while n is 2^k. This means that $n - r - 1 = 0$, and the above s^2 therefore has no meaning. The reason is that we estimate 2^k parameters (including β_0) while we have the same number of observations. This turns out to be too few observations to estimate σ^2. For intuition, this is similar to the fact that we cannot estimate σ^2 in the one-sample case if we have just one observation. (We can, however, estimate μ in this case. How?) We therefore need an alternative method for estimating σ^2.

For a full factorial experiment, MINITAB uses the so called Lenth's method (see Appendix of this note - the theory is not in the required syllabus of TMA4255). This method is based on an assumption that not all effects are non-zero, but one needs not specify which effects one suspects are zero.

In some cases a 2^k experiment is conducted with replicates, leading to two or more independent observations for each combination of low/high for the factors. In a case with r replicates of the experiment, we will have $n = r \cdot 2^k$, so SSE will have $r \cdot 2^k - 2^k = (r - 1) \cdot 2^k$ degrees of freedom. In this case the usual s^2 from regression can be used.

Without replicates, we can either use Lenth's method mentioned above, and being the default in MINITAB, or use the following method:

Estimation of σ^2 by assuming specified higher order interactions are 0

We have in general

$$\widehat{Effect}_j \sim N(Effect_j, \sigma^2_{effect})$$

This follows directly from $b_j \sim N(\beta_j, \sigma^2/n)$ (from the regression results), and then using that $\widehat{Effect}_j = 2b_j$.

It is sometimes reasonable to assume that higher order effects are 0, i.e. that the theoretical $Effect_j = 0$ when j represents such interactions, for example the interactions ABC, ABD, ACD, BCD, ABCD in a case with four factors. For such j we have

$$\widehat{Effect}_j \sim N(0, \sigma^2_{effect})$$

and hence

$$E(\widehat{Effect}_j^2) = \sigma^2_{effect}$$

Thus $\widehat{Effect}_j^2$ is an unbiased estimator of σ^2_{effect} if $Effect_j = 0$ or equivalently $\beta_j = 0$. Usually several effects are assumed to be 0, and we then use the average of the $\widehat{Effect}_j^2$ to estimate σ^2_{effect}. In the example with four factors and third and fourth order interactions assumed to be 0, we get:

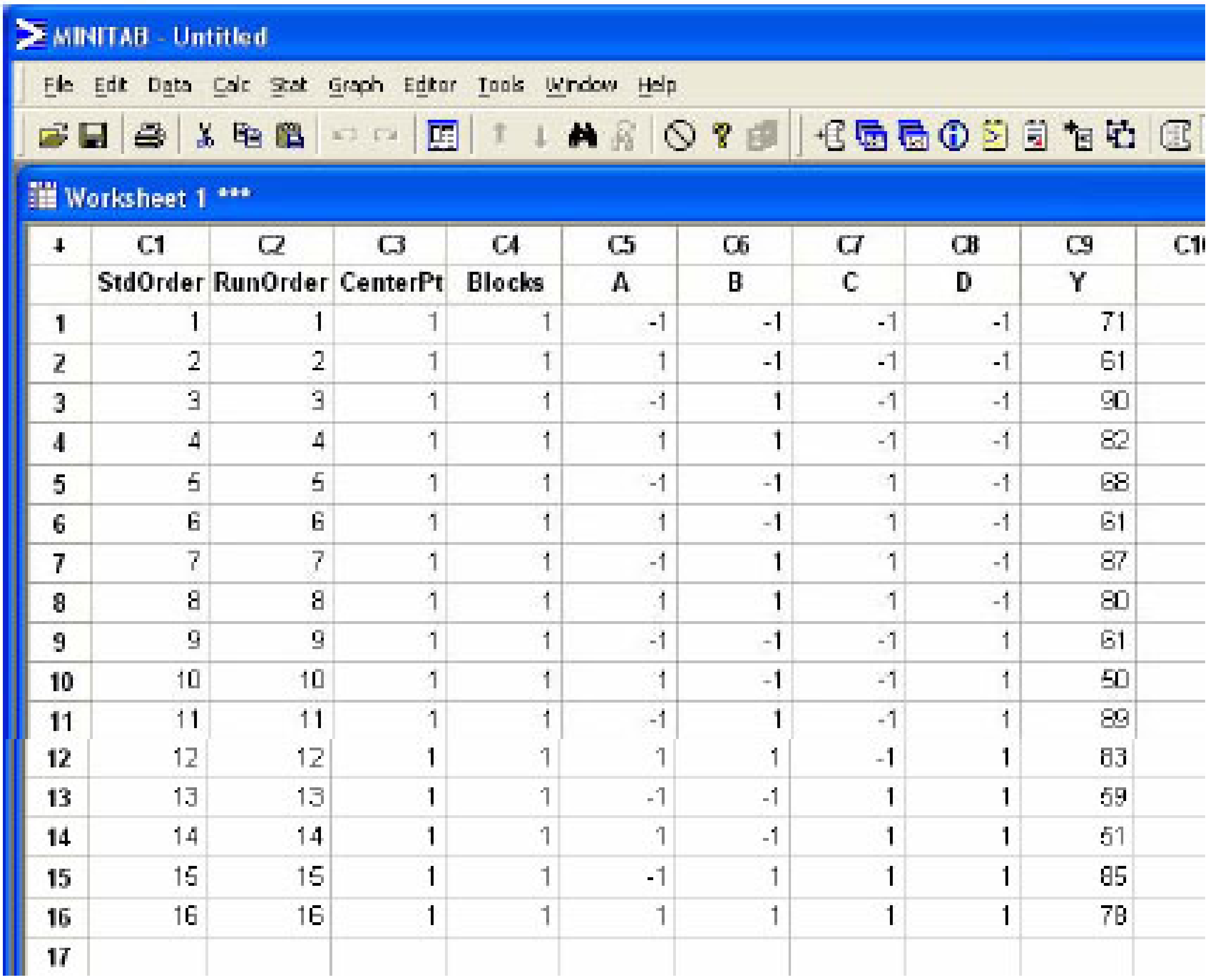
$$s^2_{effect} = \frac{\widehat{ABC}^2 + \widehat{ABD}^2 + \widehat{ACD}^2 + \widehat{BCD}^2 + \widehat{ABCD}^2}{5} \tag{5}$$

Example: Consider the setup and data in Figure 2. The effects (and coefficients) are estimated in the following output from MINITAB:

```
Factorial Fit: Y versus A; B; C; D

Estimated Effects and Coefficients for Y (coded units)

Term      Effect    Coef
Constant           72,250
A         -8,000  -4,000
B         24,000  12,000
C         -2,250  -1,125
D         -5,500  -2,750
A*B        1,000   0,500
A*C        0,750   0,375
A*D       -0,000  -0,000
B*C       -1,250  -0,625
B*D        4,500   2,250
C*D       -0,250  -0,125
A*B*C     -0,750  -0,375
A*B*D      0,500   0,250
A*C*D     -0,250  -0,125
B*C*D     -0,750  -0,375
A*B*C*D   -0,250  -0,125

S = *
```

If we assume third and fourth order interactions are 0, we can estimate σ^2_{effect} by (5), and get

$$s^2_{effect} = \frac{(-0.75)^2 + 0.5^2 + (-0.25)^2 + (-0.75)^2 + (-0.25)^2}{5} = 0.3 \tag{6}$$



↓	C1	C2	C3	C4	C5	C6	C7	C8	C9	C10
	StdOrder	RunOrder	CenterPt	Blocks	A	B	C	D	Y	
1	1	1	1	1	-1	-1	-1	-1	71	
2	2	2	1	1	1	-1	-1	-1	61	
3	3	3	1	1	-1	1	-1	-1	90	
4	4	4	1	1	1	1	-1	-1	82	
5	5	5	1	1	-1	-1	1	-1	68	
6	6	6	1	1	1	-1	1	-1	61	
7	7	7	1	1	-1	1	1	-1	87	
8	8	8	1	1	1	1	1	-1	80	
9	9	9	1	1	-1	-1	-1	1	61	
10	10	10	1	1	1	-1	-1	1	50	
11	11	11	1	1	-1	1	-1	1	89	
12	12	12	1	1	1	1	-1	1	83	
13	13	13	1	1	-1	-1	1	1	59	
14	14	14	1	1	1	-1	1	1	51	
15	15	15	1	1	-1	1	1	1	85	
16	16	16	1	1	1	1	1	1	78	
17										

Figure 2: MINITAB worksheet for a 2^4 experiment

so $s_{\mathit{effect}} = \sqrt{0.3} = 0.55$. Note that Lenth's PSE (see slides) is 1.125 and hence seems to overestimate σ_{effect}. It is in fact well known that Lenth's PSE is usually conservative.

Alternatively, we can use the ANOVA table from this experiment to compute the estimates s and s_{effect}.

```
Analysis of Variance for Y (coded units)

Source              DF   Seq SS   Adj SS   Adj MS  F  P
Main Effects         4  2701,25  2701,25  675,313  *  *
2-Way Interactions   6    93,75    93,75   15,625  *  *
3-Way Interactions   4     5,75     5,75    1,438  *  *
4-Way Interactions   1     0,25     0,25    0,250  *  *
Residual Error       0        *        *        *
Total               15  2801,00
```

From the earlier formula (4),

$$SSR = b_1^2 \sum_{i=1}^{n} x_{1i}^2 + b_2^2 \sum_{i=1}^{n} x_{2i}^2 + \cdots + b_k^2 \sum_{i=1}^{n} x_{ki}^2,$$

we can see that each estimated effect contributes to the SSR by the amount

$$b_j^2 \sum_{i=1}^{n} x_{ji}^2 = n b_j^2 = (n/4) \cdot \widehat{\mathit{Effect}}_j^2$$

Further, from

$$SSE = SST - SSR = \sum_{i=1}^{n} (y_i - \bar{y})^2 - b_1^2 \sum_{i=1}^{n} x_{1i}^2 - \cdots - b_k^2 \sum_{i=1}^{n} x_{ki}^2$$

we can see that each time a β_j is assumed to be 0, the term $b_j^2 \sum_{i=1}^{n} x_{ji}^2$ is moved from SSR to SSE. Thus, looking at the ANOVA table above, by assuming third and fourth order interactions are 0, we obtain

$$SSE = 5.75 + 0.25 = 6$$

with $4+1 = 5$ degrees of freedom. The estimate for σ^2 is hence $s^2 = SSE/df = 6/5 = 1.2$, which implies since $n = 16$,

$$s_{\mathit{effect}}^2 = (4/n)s^2 = s^2/4 = 1.2/3 = 0.3$$

which we already have found in (6) using a slightly different (but equivalent) argument.

Statistical inference in full factorial experiments

We want to find the main effects or interactions which are significantly different from 0. This is of course equivalent to finding the coefficients β_j in the corresponding regression model which are different from 0, since we have $\mathit{Effect}_j = 2\beta_j$. More precisely we want to test hypotheses of the form

$$H_0 : \mathit{Effect}_j = 0 \text{ vs } \mathit{Effect}_j \neq 0$$

or equivalently

$$H_0 : \beta_j = 0 \text{ vs } \beta_j \neq 0$$

The standard test statistic is, if σ, and hence σ_{effect}, is known:

$$Z_j = \frac{b_j}{SE(b_j)} = \frac{b_j}{\frac{\sigma^2}{n}} \sim N(0,1) \text{ under } H_0$$

or equivalently

$$Z_j = \frac{\widehat{\mathit{Effect}}_j}{SE(\widehat{\mathit{Effect}}_j)} = \frac{\widehat{\mathit{Effect}}_j}{\sigma_{\mathit{effect}}} \sim N(0,1) \text{ under } H_0$$

We reject H_0 and say that Effect_j is significant if

$$|\widehat{\mathit{Effect}}_j| > z_{\alpha/2}\sigma_{\mathit{effect}} \equiv z_{\alpha/2} \cdot \frac{2\sigma}{\sqrt{n}}$$

If σ and hence σ_{effect} are estimated by s and s_{effect}, respectively, then we reject H_0 and say that Effect_j is significant if

$$|\widehat{\mathit{Effect}}_j| > t_{\alpha/2,\nu}s_{\mathit{effect}} \equiv t_{\alpha/2,\nu} \cdot \frac{2s}{\sqrt{n}} \tag{7}$$

where ν is the number of degrees of freedom connected to the estimates of σ and σ_{effect} that are used. When Lenth's PSE is used, the degrees of freedom is

$$df = \frac{2^k - 1}{3}$$

where $2^k - 1$ is the number of effects in the model, while the 3 in the denominator has been found empirically by Lenth.

Graphics in MINITAB

The slides show Pareto plots and normal plots obtained from MINITAB.

The Pareto plots are graphs of the $|\widehat{\mathit{Effect}}_j|$, displayed in decreasing order of magnitude. The indicated critical value is the right hand side of (7).

The normal plot in MINITAB is constructed in the same manner as the normal plot that was considered earlier in the course. The straight line corresponds to the distribution $N(0, s^2_{\mathit{effect}}$. Thus, effects that are not significant are supposed to fall close to the line, while significant effects will fall outside the line (positve effects to the right, negative effects to the left).

MINITAB also provides cube plots like the one depicted in Figure 3 for the Three factors data.

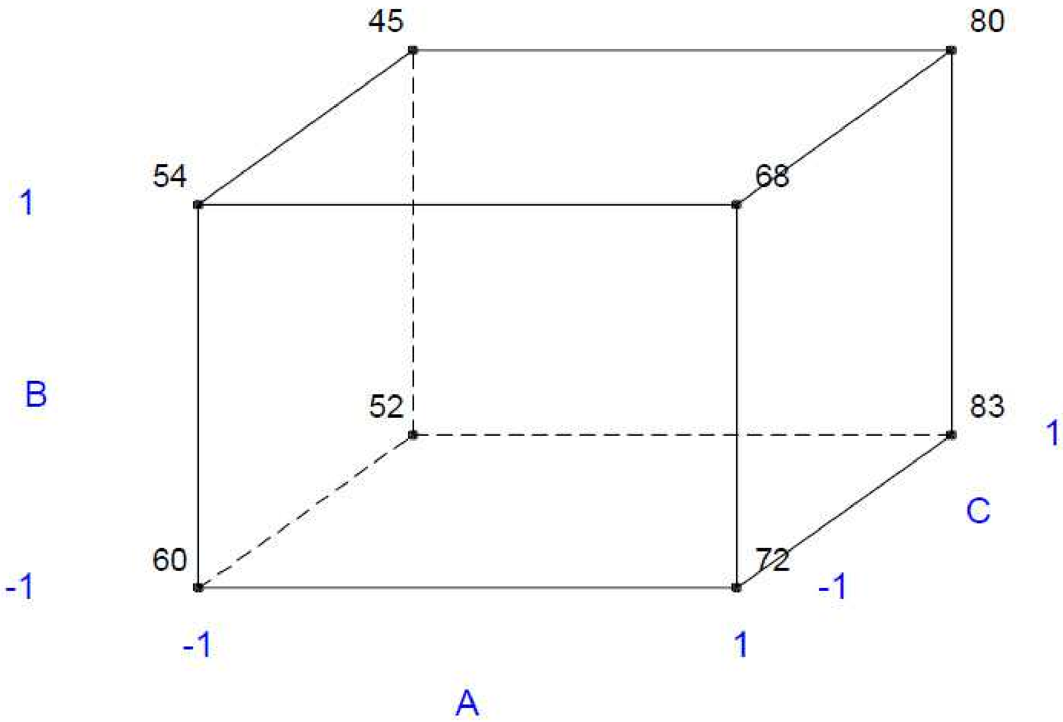


Figure 3: Cube plot of data in the table for Three factors

Blocking in 2^k experiments

The individual experiments of a 2^k experiment should always be done in randomized order. (MINITAB does this randomization for us). Randomization is our best guarantee for independent observations, and implies less chances that external factors influence the response, which may lead to wrong conclusions. It is also important to check and adjust all level combinations between each individual experiment. This is to assure as much as possible equal variances.

If many experiments are to be performed it may still happen that external conditions vary from beginning to end of the total experiment. Such changes of conditions may affect responses and hence again lead to wrong conclusions. To avoid such effects we may perform the experiment in blocks. Sometimes there are also other concerns, for example shortage of raw material, that forces one to block divide an experiment. When an experiment is divided into blocks, we should randomize within the blocks.

Example: 2^3 experiment in two blocks

The idea is to use the column for ABC to define the blocks. Block I corresponds to the combinations with $-$ in ABC, while Block II has $+$ in this column. Thus we get:

St. order	A	B	C	AB	AC	BC	Block	ABC
1	-	-	-	+	+	+	I	-
4	+	+	-	+	-	-	I	-
6	+	-	+	-	+	-	I	-
7	-	+	+	-	-	+	I	-
2	+	-	-	-	-	+	II	+
3	-	+	-	-	+	-	II	+
5	-	-	+	+	-	-	II	+
8	+	+	+	+	+	+	II	+

We observe that if an amount h is added to the responses of all single experiments in Block II, while nothing is added to the responses of Block I, then computation of main effects and two factor interactions is not affected. This is not the case for the three-factor interaction, however, which will be so-called *confounded* with the block effect.

Example: 2^3 experiment in four blocks

We will now need *two* columns of the full experiment to define the four blocks. Suppose we use the two-factor interactions AB and BC to define the blocks. The blocks are determined as follows:

Block I AB has $-$, BC has $-$

Block II AB has $-$, BC has $+$

Block III AB has $+$, BC has $-$

Block IV AB has $+$, BC has $+$

This gives:

St. order	A	B	C	AB	AC	BC	Block	ABC
3	-	+	-	-	+	-	I	+
6	+	-	+	-	+	-	I	-
2	+	-	-	-	-	+	II	+
7	-	+	+	-	-	+	II	-
4	+	+	-	+	-	-	III	-
5	-	-	+	+	-	-	III	+
1	-	-	-	+	+	+	IV	-
8	+	+	+	+	+	+	IV	+

It is clear that the interactions AB, BC, AC are all confounded with the block effect (and can therefore not be estimated). The three main effects, may however be estimated, and in fact the third order interaction ABC is also not confounded with the blocks.

How can we decide which columns to use for blocking?

We will always try to block in such a manner that we may estimate main effects and possibly low-order interactions. Let I be a column of only +. (Do not confuse it with the roman number I used in the tables above). Then

$$I = AA = BB = CC$$

where columns are multiplied elementwise (++ is +, +- is - etc.)

Assume that a 2^3 experiment is block divided following the columns $D = ABC$ and $E = AC$. The interaction between D and E is $DE = ABCAC = AABCC = B$. It follows that the main effect of B is confounded with the block effect, in addition to ABC and BC. It is therefore better to divide according to AB and BC as we did above. This is because then the interaction between AB and BC is AC (which is not a main effect!)

Appendix

Estimation of $\sigma_{\textit{effect}}$ by Lenth's method: The Pseudo Standard Error

Let $C_1, C_2, \ldots, C_m$ be estimated effects, e.g. $\hat{A}, \hat{B}, \widehat{AB}$, etc.

1. Order absolute values $|C_j|$ in increasing order.
2. Find the median of the $|C_j|$ and compute preliminary estimate
$$s_0 = 1.5 \cdot \text{median}_j |C_j|$$
3. Take out the effects C_j with $|C_j| \geq 2.5 \cdot s_0$ and find the median of the rest of the $|C_j|$. Then PSE is this median multiplied by 1.5, i.e.
$$\text{PSE} = 1.5 \cdot \text{median}\{|C_j| : |C_j| < 2.5 s_0\}$$
and this is Lenth's estimate of $\sigma_{\textit{effect}}$.
4. Lenth has suggested empirically that the degrees of freedom to be used with PSE is $m/3$ where m is the initial number of effects in the algorithm. Thus we claim as significant the effects for which $|C_j| > t_{\alpha/2, m/3} \cdot PSE$.

Example with Three factors

There are $m = 7$ estimated effects.

1. Ordered estimated absolute effects:
$$0, 0.5, 1.5, 1.5, 5, 10, 23$$
2. Median is 1.5 so $s_0 = 1.5 \cdot 1.5 = 2.25$.
3. Throw out large effects, i.e. the ones that are
$$\geq 2.5 \cdot 2.25 = 5.625$$
leaving us with $0, 0.5, 1.5, 1.5, 5$ for which median is still 1.5, so
$$\text{PSE} = 1.5 \cdot 1.5 = 2.25$$
4. Lenth's degrees of freedom is $m/3 = 7/3 = 2.33$, so we claim effects to be significant at 5% level when
$$|C_j| > t_{0.025, 2.33} \cdot 2.25 = 3.765 \cdot 2.25 = 8.47.$$

Some theoretical considerations

- The basic underlying idea is that many of the true effects are zero, and that (most of) the ones that are not zero are thrown out in the last step of the algorithm.

- The reason for 1.5 is that if $C \sim N(0, \sigma^2_{effect})$ then the median of the distribution of $|C|$ is $0.675\sigma_{effect}$, so that the median of the distribution of $1.5 \cdot |C|$ is
$$1.5 \cdot 0.675\sigma_{effect} \approx \sigma_{effect}.$$